

Technical University of Denmark



## Modelling Framework for the Identification of Critical Variables and Parameters under Uncertainty in the Bioethanol Production from Lignocellulose

Morales Rodriguez, Ricardo; Meyer, Anne S.; Gernaey, Krist V.; Sin, Gürkan

*Publication date:*  
2011

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*

Morales Rodriguez, R., Meyer, A. S., Gernaey, K., & Sin, G. (2011). Modelling Framework for the Identification of Critical Variables and Parameters under Uncertainty in the Bioethanol Production from Lignocellulose. Poster session presented at AMIDIQ 32nd National Meeting and 1st International Congress, Riviera Maya, Mexico.

**DTU Library**  
Technical Information Center of Denmark

---

**General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Modelling Framework for Identification of Critical Variables and Parameters under Uncertainty in the Bioethanol Production from Lignocellulose

<sup>1</sup>Ricardo Morales-Rodriguez, <sup>2</sup>Anne S. Meyer, <sup>3</sup>Krist V. Gernaey, <sup>1</sup>Gürkan Sin  
<sup>1</sup>CAPEC, <sup>2</sup>Center of Bioprocess Engineering, <sup>3</sup>Center of Process Engineering and Technology, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

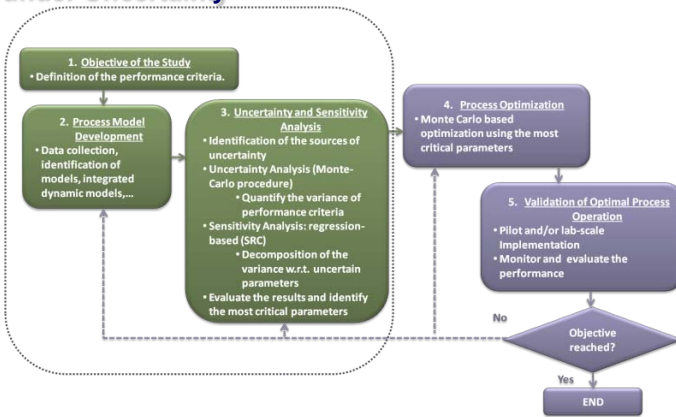
## I. Introduction

This study presents the development of a systematic modelling framework for identification of the most critical variables and parameters under uncertainty, evaluated on a lignocellulosic ethanol production case study. The systematic framework starts with: (1) definition of the objectives; (2) Collection of data and the implementation of dynamic models for each unit operation in the process; (3) Uncertainty and sensitivity analysis, performed to identify the critical operational variables and parameters in the process. The uncertainty and sensitivity analysis identified the following most critical variables and parameters involved in the lignocellulosic ethanol production case study. For the operating cost, the enzyme loading showed the strongest impact, while reaction volume showed a significant impact on the ethanol/biomass ratio. The results showed also that it is possible to find a better alternative operation of the plant in comparison with the base case.

## II. Objective:

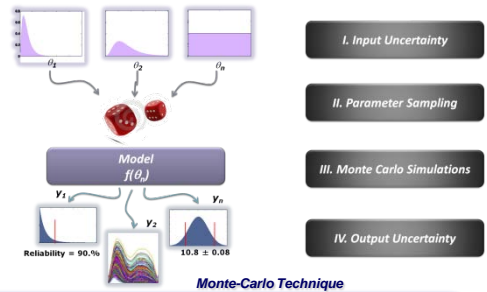
Develop a systematic framework for the identification of the most critical variables and parameter of bioprocesses subject to various sources of uncertainties.

## III. Systematic Framework for Bioprocess Identification under Uncertainty



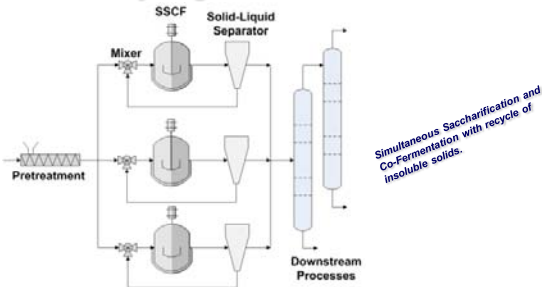
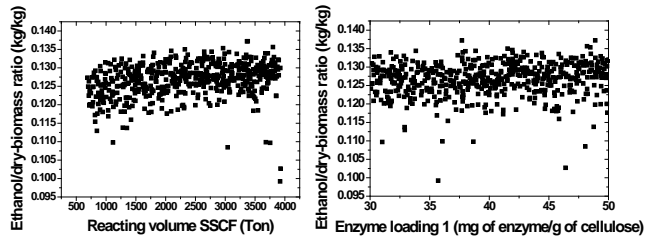
## IV. Uncertainty and Sensitivity Analysis

The uncertainty analysis is carried out using the Monte-Carlo technique. Sensitivity analysis employs the standardized regression coefficient (SRC) method, which provides a global sensitivity measure,  $\beta_i$ , thereby showing how much each parameter contributes to the variance (uncertainty) of the model predictions.



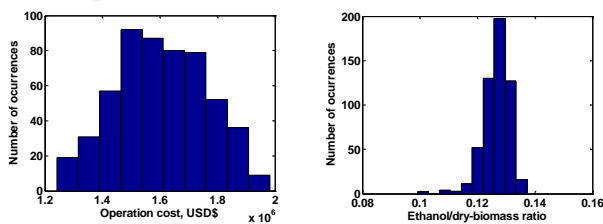
## V. Case Study: Lignocellulosic Ethanol Production

### V.c Correlation among Parameters and Performance Criteria

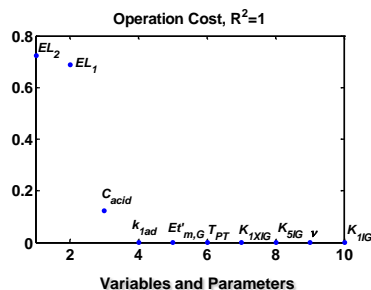


(Morales-Rodriguez, et al., 2011, *Bioresour. Technol.* (102) 1174-1184.)

### V.a Averaged Plant Performance from Monte-Carlo Simulation



### V.b Influence of Parameters and Variables in the Operating Cost



## VI. Discussion and Concluding Remarks

- A systematic framework for identification of the most critical parameters and operation variables under uncertainty has been introduced.
- Employing a bioethanol process flowsheet, the operating cost and the enzyme loading showed the strongest impact, while reaction volume showed a significant impact on the ethanol/biomass ratio.
- The results showed also that it is possible to find a better alternative operation of the plant in comparison with the base case.

## Acknowledgment



Mexican National Council for Science and Technology (CONACYT). Project # 145066.